

Appl. No. : 09/919,739
Filed : July 31, 2001

REMARKS

By this Amendment, Claims 3, 6, and 7 are amended and Claim 5 is canceled. The preamble of Claim 3 has been amended to include "constructing a model for predicting molecular behavior using marker molecules." Support for this amendment can be found, for example, on page 5, lines 10-11 of the specification. Claim 3 has also been amended to include the step of "receiving data related to one or more chemical or biological properties of a set of structurally defined reference molecules." Support for this amendment can be found, for example, on page 4, lines 18-21; page 5, lines 19-31; and page 14, lines 3-15 of the specification. Other amendments to Claim 3 incorporate limitations previously found in Claim 5.

Claim 6 has been amended so that it no longer depends on canceled Claim 5. Claim 7 has been amended so that it depends on Claim 3 and to incorporate limitations previously found in Claim 5. Claims 3-4 and 6-8 remain pending.

Objection

The Examiner has objected to Claim 3 because an "e" was missing from the word "one" as originally filed. The Applicants respectfully submit that the present amendment adding an "e" overcomes the objection.

Rejections Under § 101

The examiner has rejected Claims 3-8 as being directed to non-statutory subject matter. The Applicants respectfully submit that, as amended, Claims 3-4 and 6-8 are directed to statutory subject matter because they disclose processes that are limited to practical applications in the technological arts and they disclose manipulating data representing physical objects.

The preamble of Claim 3 has been amended to more clearly indicate that the claimed process produces a "model for predicting molecular behavior using marker molecules." Claimed subject matter is statutory if "the claimed process" is "limited to a practical application of" a "mathematical algorithm in the technological arts" (M.P.E.P. § 2106(IV)(B)(2)(b)(ii)). "A claim is limited to a practical application when the method, as claimed, produces a concrete, tangible and useful result" (M.P.E.P. § 2106(IV)(B)(2)(b)(ii)). The method of Claim 3 produces a concrete, tangible, and useful result, namely a model for predicting the behavior of molecules

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that have not yet been physically tested. As such, Claims 3-4 and 6-8 are directed to statutory subject matter.

Claim 3 has also been amended to recite “receiving data related to one or more chemical or biological properties of a set of structurally defined reference molecules.” The structure and the chemical and biological properties of the reference molecules are measurements of physical objects. Such data must be obtained from the physical world. These are real molecules that exist and have been synthesized and characterized. In other words, if Claim 3 is being implemented as an algorithm in a computer system, the algorithm itself cannot calculate the “one or more chemical or biological properties.” In contrast, the step in Claim 3 of “classifying the respective molecules in said set of reference molecules as either possessing or not possessing at least one property” could be performed in a computer algorithm. For example, at the bottom of page 5 in the specification, a sample set of reference molecules is provided. The property of “% protein bound” comes from the physical world and is not calculated by a computer algorithm. On the other hand, the classification of having “high protein binding” or not could be determined by a computer algorithm once the percent protein bound data is transformed into computer data. Therefore, Claims 3-4 and 6-8 require the “manipulation of data representing physical objects” and therefore are directed to statutory subject matter (M.P.E.P. § 2106(IV)(B)(2)(b)(i)).

Rejections Under § 112

The Examiner has rejected Claims 5-8 as lacking support in the specification for the limitation of “repeating...for at least some other molecules of said subset.” The Applicants have canceled Claim 5. It is respectfully submitted that Claims 6-8 are allowable.

Rejections Under § 102

The Examiner has rejected Claims 3-8 as allegedly being anticipated by Stanton et al. The Applicants respectfully submit that Stanton et al. does not anticipate any of Claims 3-4 and 6-8 as amended. With respect to independent Claim 3, at a minimum, Stanton et al. does not disclose the steps of “defining...a fractions-correctly-predicted metric,” “counting the number of molecules...,” and “choosing said first molecule as a marker molecule...”

Claim 3 further requires “sorting” molecules “in descending order of numerical similarity” from a “first molecule.” The Examiner has alleged that the squared Euclidean

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distance similarity metric disclosed in Stanton et al. reads on the “similarity metric” of now amended Claim 3 (previously a limitation in Claim 5; see 9/22/03 Office Action, page 7). In addition, the Examiner has alleged that the disclosure in Stanton et al. of sorting molecules in descending order of numerical similarity based on Euclidean distance reads on the “sorting” step in now amended Claim 3 (previously a limitation in Claim 5; see 9/22/03 Office Action, page 8). The Examiner goes on to allege that the last column of Table 2 in Stanton et al., titled “hit rate as a % of compds tested,” reads on the “fractions-correctly-predicted metric” in now amended Claim 3 (previously a limitation in Claim 5; see 9/22/03 Office Action, pages 8-9).

The Applicants respectfully disagrees with the Examiner’s analysis. Claim 3 explicitly defines the “fractions-correctly-predicted metric as the number of molecules in said range which are also members of said subset divided by the total number of molecules in said range.” The “range” in this limitation is the “range in molecules of similarity distance away from” the “first molecule.” In contrast, Stanton et al. does not disclose similarity distances in Table 2, let alone a range of similarity distances. Instead, Table 2 discloses the hit percent for *all* compounds returned in the nearest neighbor search for each of the eleven disclosed examples. Figure 5b plots the hit percent for the *combination* of molecules from *all* eleven examples as a function of nearest neighbor Euclidean distance; however, Figure 5b does not disclose the hit percent as a function of nearest neighbor distance for each independent example. In other words, Stanton et al. does not disclose, nor is it possible to determine from Table 2 or Figure 5b, hit percents of the nearest neighbors to *one* of the eleven particular original queries (“a first molecule”). Furthermore, the hit percent in Stanton et al. is the hit percent for the molecules tested that have a *given nearest neighbor distance* from the original query. Figure 5b does not report, nor is it disclosed elsewhere in Stanton et al., the hit percent for *all* molecules within the *range* between the original query and a given nearest neighbor distance. Thus, Stanton et al. does not disclose the “fraction-correctly-predicted metric” as defined in Claim 3, and therefore does not anticipate Claim 3.

Moreover, Stanton et al. does not disclose the step of “counting the number of molecules away from said first molecule at which the fractions-correctly-predicted metric for said first molecule drops below a threshold value.” The Examiner has pointed out that Stanton et al. discloses that the 20-30 closest neighbors to a given query were selected for subsequent purchase and screening (see 9/22/03 Office Action, page 8). However, merely selecting a number of

closest neighbors without a specified criteria for the selection cannot meet the limitations of Claim 3, which require counting the number of molecules when “the fractions-correctly-predicted metric for said first molecule drops below a threshold value.” In contrast to this specified criteria, Stanton et al. states with respect to the 20-30 closest neighbors that “[i]nitially, this number was chosen arbitrarily” (page 22, col. 1, line 6). Furthermore, Stanton et al. merely discloses selecting nearest neighbors and does not disclose “counting.” The Examiner has also pointed out that Stanton et al. discloses that a 20 percent hit rate may be obtained by considering only the available compounds within a nearest neighbor distance of 1.9 or less (9/22/03 Office Action, page 9; Stanton et al., page 26, col. 2, lines 9-11). However, as discussed above, the hit rate in Stanton et al. is not the same as the claimed “fractions-correctly-predicted metric.” Furthermore, Stanton et al. does not call for counting the number of molecules within a nearest distance of 1.9 to the original query, nor is that number provided. Indeed, it would not be possible to determine the count from the information plotted in Figure 5, because Figure 5 combines data from *all* 11 examples in Table 2. As such, counts of molecules at given nearest neighbor distances from a particular original query (“a first molecule”) are not plotted. Thus, Stanton et al. does not disclose the “counting” step of Claim 3 and, for this additional reason, does not anticipate Claim 3.

Stanton et al. also does not disclose the limitation of the “choosing” step in Claim 3. Claim 3 requires “choosing said first molecule as a marker molecule if said first molecule has a fractions-correctly-predicted metric which exceeds said threshold value for a pre-selected minimum distance.” Stanton et al. discloses calculating hit percents for nearest neighbor searches on original queries (Stanton et al, Table 2 and Figure 5b). As discussed above, these hit percents are not the same as the “fractions-correctly-predicted metric.” Furthermore, Stanton et al. does not disclose choosing particular original queries based on the hit percents for a pre-selected minimum distance. The disclosure in Stanton et al., of a set of original query examples for which the *combined* data indicated a 20% hit rate within a nearest neighbor distance of 1.9, was not used as a criteria for choosing certain of the original queries over others. Since the “choosing” step is not at all disclosed in Stanton et al., for this additional reason Claim 3 is not anticipated by Stanton et al.

It is also worth noting the difference between Claim 3 as a whole and Stanton et al. The Examiner has alleged that finding hits within a large combinatorial library as disclosed in Stanton

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et al. reads on the “classifying” step of Claim 3 (9/22/03 Office Action, pages 6-7). Thus, the Examiner has argued that the large combinatorial library disclosed in Stanton et al. reads on the “set of reference molecules” of Claim 3. Furthermore, the Examiner has alleged that performing hierarchical cluster analysis to obtain subsets of hits as disclosed in Stanton et al. reads on the “subset” of Claim 3. If these allegations were correct, Claim 3 would require, among other steps, “selecting a first molecule” from a “subset” created in the hierarchical cluster analysis and sorting all of the molecules from the “set” of the large combinatorial library “in descending order of numerical similarity.” However, in Stanton et al., Figure 5 only depicts Euclidean distances from original query compounds for the compounds returned in nearest neighbor searches, not the entire combinatorial library of compounds. Furthermore, as discussed above, Stanton et al. does not disclose choosing particular original queries used in nearest neighbor searches. Thus, Claim 3 as a whole is not disclosed in Stanton et al. See M.P.E.P. § 2106(II)(C): “[W]hen evaluating the scope of a claim, every limitation in the claim must be considered. Office personnel may not dissect a claimed invention into discrete elements and then evaluate the elements in isolation. Instead, the claim as a whole must be considered.” (emphasis in original).

Claim 4, 6, and 7 depend from Claim 3, and Claim 8 depends from Claim 7. Therefore, for at least the same reasons as Claim 3, Claims 4 and 6-8 are not anticipated by Stanton et al. Furthermore, Claim 7 requires a “repeating” step using “a plurality of different threshold values and minimum distances.” Stanton et al. does not disclose the use of multiple threshold values for a “fractions-correctly-predicted metric”; nor does it disclose the use of multiple minimum nearest neighbor distances. Thus, for this additional reason, Stanton et al. does not anticipate Claims 7 and 8.

CONCLUSION

The Applicants have amended the claims in order to address the Examiner’s objection and rejections based on sections 101, 112, and 102. The applicants respectfully submit that all of the rejections have been overcome and the cited art distinguished. As such, allowance of all pending claims is respectfully requested.

If the Examiner has any questions that may be answered by telephone, she is invited to call the undersigned directly.

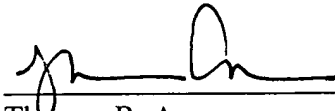
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Please charge any additional fees, including any fees for additional extension of time, or credit overpayment to Deposit Account No. 11-1410.

Respectfully submitted,

KNOBBE, MARTENS, OLSON & BEAR, LLP

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By: 
Thomas R. Arno
Registration No. 40,490
Attorney of Record
Customer No. 20,995
(619) 235-8550

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